

Markov substitute processes : a new model for linguistics and beyond

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March 28, 2016

Abstract

We introduce Markov substitute processes, a new model at the crossroad of statistics and formal grammars, and prove its main property : Markov substitute processes with a given support form an exponential family.

Keywords : Markov processes, Natural language processing, Statistical models for finite state processes.

MSC 2010 classification 62M09, 60J10, 91F20, 68T50,

1 Introduction

We defined in a previous work [Mainguy, 2014] Markov substitute models with linguistics in mind [Stabler, 2009, Roark, 2001]. Our purpose was to propose families of probability measures on sentences (finite sequences of words taken from a given finite dictionary), and use them to learn the syntax of a language from an i.i.d. random sample of sentences by performing some suitable kind of statistical estimation. However, the model we built with this idea in mind turned out to be a general purpose extension of Markov chains that can be applied to other types of data.

2 Definition of Markov substitute models

According to our definition, a Markov substitute model is a family of probability measures on finite sequences of words taken from a finite dictionary D . Therefore, the state space of the model is $D^+ = \bigcup_{j=1}^{\infty} D^j$, the set of all sentences of finite non-zero length. Adding the empty string ε of zero length, we will also consider $D^* = \{\varepsilon\} \cup D^+$.

In a Markov substitute model, some expressions (subsequences of words) can be substituted to others independently from the context. To give a precise definition of this property, it is useful to introduce the insertion operator α . It operates on a two sided context $x = (x_1, x_2) \in D^* \times D^*$, (where the left and right contexts x_1 and x_2 may be empty strings), and an expression $y \in D^+$ (that is a non-empty finite string of words). The insertion operator is defined as

$$\alpha(x, y) = \gamma(x_1, y, x_2), \quad x \in D^* \times D^*, y \in D^+,$$

where γ is the concatenation operator that simply pieces strings together. Remark that given $x \in (D^*)^2$, the map

$$\begin{aligned} D^+ &\rightarrow D^+ \\ y &\mapsto \alpha(x, y) \end{aligned}$$

is one to one, whereas for a given $y \in D^+$, the map

$$\begin{aligned} (D^*)^2 &\rightarrow D^+ \\ x &\mapsto \alpha(x, y) \end{aligned}$$

is not, since, for instance, $\gamma(y, y, y') = \alpha((y, y'), y) = \alpha[(\varepsilon, \gamma(y, y')), y]$.

We define Markov substitute models in terms of Markov substitute sets.

Definition 2.1

Consider a domain $\mathcal{D} \subset D^+$ (that may be D^+ itself or any subset of it). Consider a probability distribution $P \in \mathcal{M}_+^1(D^+)$ on nonempty strings of words, such that $\text{supp}(P) \subset \mathcal{D}$. Introducing the domain \mathcal{D} allows for instance to impose if needed that P has a finite support. The support of P defines a language (a subset of non empty strings of words), and P itself indicates the probability to observe any given sentence in this language. A set $B \subset D^+$ of syntagms is called a Markov substitute set of the string distribution P if and only if there exists a skew-symmetric function $\beta : B \times B \rightarrow \mathbb{R}$, called a substitute exponent, such that for any context $x \in (D^*)^2$ and any $y, y' \in B$, such that $\{\alpha(x, y), \alpha(x, y')\} \subset \mathcal{D}$,

$$P(\alpha(x, y')) = P(\alpha(x, y)) \exp(\beta(y, y')). \quad (2.1)$$

(By skew symmetric, we mean that $\beta(y, y') = -\beta(y', y)$.) We chose the notation β instead of β_B , because in the case when $\{y, y'\} \subset B \cap B'$, the intersection of two Markov substitute sets, the substitute exponents involved in the property that B is a Markov substitute set and in the property that B' is a Markov substitute set are the same when the pair $\{y, y'\}$ is active, meaning that there is $x \in (D^*)^2$, such that $P(\alpha(x, y)) > 0$ and $P(\alpha(x, y')) > 0$ and are arbitrary and therefore can also be chosen to be the same when the pair $\{y, y'\}$ is not active.

Proposition 2.1

For any Markov substitute set B of P on the domain \mathcal{D} , for any $x_1, x_2 \in (D^*)^2$ and any $y_1, y_2 \in B$ such that $\{\alpha(x_i, y_j), 1 \leq i \leq 2, 1 \leq j \leq 2\} \subset \mathcal{D}$,

$$P(\alpha(x_1, y_1))P(\alpha(x_2, y_2)) = P(\alpha(x_1, y_2))P(\alpha(x_2, y_1)). \quad (2.2)$$

This proposition shows that we can exchange y_1 and y_2 in a pair of independent draws from P without changing the likelihood of this pair. This generalizes of course to larger i.i.d. samples drawn from P : we do not change the likelihood of the sample if we exchange y_1 and y_2 belonging to the same Markov substitute set B .

PROOF. Using the definition, we see that

$$\begin{aligned} P(\alpha(x_1, y_1))P(\alpha(x_2, y_2)) \\ &= P(\alpha(x_1, y_2)) \exp(\beta(y_2, y_1)) P(\alpha(x_2, y_1)) \exp(\beta(y_1, y_2)) \\ &= P(\alpha(x_1, y_2))P(\alpha(x_2, y_1)). \quad \square \end{aligned}$$

Markov substitute sets have the following elementary properties.

Proposition 2.2

- A subset of a Markov substitute set is itself a Markov substitute set.

- A set $B \subset D^+$ is a Markov substitute set if and only if, for any $y, y' \in B$, the pair $\{y, y'\}$ is a Markov substitute set.
- If $B \subset D^+$ is a Markov substitute set and if $x \in (D^*)^2$ then

$$\alpha(x, B) \stackrel{\text{def}}{=} \{\alpha(x, y), y \in B\}$$

is also a Markov substitute set.

PROOF. The first points are straightforward consequences of eq. (2.1). As for the last point, writing $x = (x_1, x_2)$, where $x_1, x_2 \in D^*$, we see by the definitions that for any $(z_1, z_2) \in (D^*)^2$ and any $y, y' \in B$, such that $\{\alpha(z, \alpha(x, y)), \alpha(z, \alpha(x, y'))\} \subset \mathcal{D}$,

$$\begin{aligned} \mathbb{P}[\alpha(z, \alpha(x, y'))] &= \mathbb{P}[\alpha(\gamma(z_1, x_1), \gamma(x_2, z_2), y')] \\ &= \mathbb{P}[\alpha(\gamma(z_1, x_1), \gamma(x_2, z_2), y)] \exp(\beta(y, y')) = \mathbb{P}[\alpha(z, \alpha(x, y))] \exp(\beta(y, y')), \end{aligned}$$

proving that $\alpha(x, B)$ is a Markov substitute set with substitute exponent

$$\beta(\alpha(x, y), \alpha(x, y')) = \beta(y, y'), \quad y, y' \in B. \quad \square$$

Definition 2.2

For any given family \mathcal{B} of subsets of D^+ , we will say that the random process $S \in D^+$ is a \mathcal{B} -Markov substitute process on the domain \mathcal{D} if and only if all the members of \mathcal{B} are Markov substitute sets of its probability distribution \mathbb{P}_S . We will say that the probability distribution \mathbb{P}_S of S is a \mathcal{B} -Markov substitute probability measure on \mathcal{D} . We will use the notation $\mathfrak{M}(\mathcal{D}, \mathcal{B})$ to denote the set of \mathcal{B} -Markov substitute probability measures on \mathcal{D} .

3 Markov substitute processes as exponential families

To describe the possible supports of \mathcal{B} -Markov substitute processes, we introduce the equivalence relation $\sim_{\mathcal{B}}$ on \mathcal{D} that is the smallest one such that, for any $x \in (D^*)^2$, $y, y' \in B \in \mathcal{B}$, such that $\alpha(x, \{y, y'\}) \subset \mathcal{D}$,

$$\alpha(x, y) \sim_{\mathcal{B}} \alpha(x, y').$$

In other words, $\mathcal{D}/\sim_{\mathcal{B}}$ are the connected components of the graph

$$\mathcal{G}(\mathcal{D}, \mathcal{B}) = \left\{ (\alpha(x, y), \alpha(x, y')), x \in (D^*)^2, y, y' \in B \in \mathcal{B} \right\} \cap (\mathcal{D} \times \mathcal{D}). \quad (3.1)$$

It turns out that for any domain $\mathcal{D} \subset D^+$ and any family \mathcal{B} of subsets of D^+ , $\mathfrak{M}(\mathcal{D}, \mathcal{B}) \neq \emptyset$. To prove this, it will be useful to introduce the special family of independent Markov substitute processes. Given a strict sub-probability measure $\xi \in \mathcal{M}_+(D)$, let us put

$$r = 1 - \sum_{w \in D} \xi(w) > 0,$$

and let us define the independent process \tilde{S}_ξ by its distribution

$$\mathbb{P}(\tilde{S}_\xi = w_{1:k}) = \frac{r}{1-r} \prod_{j=1}^k \xi(w_j).$$

Let us remark that $\mathbb{P}[\ell(\tilde{S}_\xi) = L] = r(1-r)^{L-1}$. It is easy to see from the definition that $\text{supp}(\xi)^+ = \text{supp}(\tilde{S}_\xi)$ is a Markov substitute set of the independent Markov substitute process \tilde{S}_ξ and that its substitute exponent is equal to

$$\beta(y, y') = \log \left(\frac{\mathbb{P}(\tilde{S}_\xi = y')}{\mathbb{P}(\tilde{S}_\xi = y)} \right), \quad y, y' \in \text{supp}(\xi)^+.$$

Proposition 3.1

For any domain \mathcal{D} and any family \mathcal{B} of subsets of D^+ , for any \mathcal{B} -Markov substitute measure \mathbb{P} on \mathcal{D} , there is a subset $\mathcal{C}_\mathbb{P} \subset \mathcal{D}/\sim_\mathcal{B}$ of components of \mathcal{D} such that the support $\text{supp}(\mathbb{P})$ is of the form

$$\text{supp}(\mathbb{P}) = \bigcup_{C \in \mathcal{C}_\mathbb{P}} C. \quad (3.2)$$

Conversely, for any subset $\mathcal{C} \subset \mathcal{D}/\sim_\mathcal{B}$ of components of \mathcal{D} , any strict sub-probability measure $\xi \in \mathcal{M}_+(D)$, such that $\text{supp}(\xi) = D$, and any probability measure $\mu \in \mathcal{M}_+^1(\mathcal{D}/\sim_\mathcal{B})$, such that $\text{supp}(\mu) = \mathcal{C}$, the probability measure on \mathcal{D} defined as

$$\mathbb{P}(s) = \sum_{C \in \mathcal{C}} \mathbb{1}(s \in C) \mu(C) \mathbb{P}(\tilde{S}_\xi = s \mid \tilde{S}_\xi \in C), \quad s \in \mathcal{D}, \quad (3.3)$$

is a \mathcal{B} -Markov substitute measure on the domain \mathcal{D} with support

$$\text{supp}(\mathbb{P}) = \bigcup_{C \in \mathcal{C}} C. \quad (3.4)$$

PROOF. Let

$$\mathcal{C}_\mathbb{P} = \{C \in \mathcal{D}/\sim_\mathcal{B}; \mathbb{P}(C) > 0\},$$

so that obviously $\text{supp}(\mathbf{P}) \subset \bigcup_{C \in \mathcal{C}_P} C$. Conversely, for any $C \in \mathcal{C}_P$, there is $s_C \in C$ such that $\mathbf{P}(s_C) > 0$. By definition of $\mathcal{D}/\sim_{\mathcal{B}}$, for any $s \in C \in \mathcal{C}_P \in \mathcal{D}/\sim_{\mathcal{B}}$, there are finite sequences

$$\begin{aligned} s_k &\in C, & 0 \leq k \leq \ell, \\ x_k &\in (D^*)^2, & 1 \leq k \leq \ell, \\ B_k &\in \mathcal{B}, & 1 \leq k \leq \ell, \\ (y_k, y'_k) &\in B_k^2, & 1 \leq k \leq \ell, \end{aligned}$$

such that $s_0 = s_C$, $s_\ell = s$, $s_{k-1} = \alpha(x_k, y'_k)$ and $s_k = \alpha(x_k, y_k)$, $1 \leq k \leq \ell$. Consequently

$$\mathbf{P}(s) = \mathbf{P}(s_C) \prod_{k=1}^{\ell} \exp(\beta(y'_k, y_k)) > 0,$$

so that $C \subset \text{supp}(\mathbf{P})$. Therefore $\bigcup_{C \in \mathcal{C}_P} C \subset \text{supp}(\mathbf{P})$, proving eq. (3.2).

Let us now come to the second part of the proposition. The support of \tilde{S}_ξ being D^+ , it is clear that the support of S defined by eq. (3.3) is the one defined by eq. (3.4). For any $B \in \mathcal{B}$, let us define

$$\beta(y, y') = \log \left(\frac{\mathbf{P}(\tilde{S}_\xi = y')}{\mathbf{P}(\tilde{S}_\xi = y)} \right), \quad y, y' \in B.$$

For any $B \in \mathcal{B}$, any $x \in (D^*)^2$, any $y, y' \in B$, such that $\alpha(x, \{y, y'\}) \subset \mathcal{D}$, there is $C \in \mathcal{D}/\sim_{\mathcal{B}}$ such that $\alpha(x, \{y, y'\}) \subset C$ and

$$\begin{aligned} \mathbf{P}(\alpha(x, y')) &= \frac{\mu(C) \mathbf{P}(\tilde{S}_\xi = \alpha(x, y'))}{\mathbf{P}(\tilde{S}_\xi \in C)} \\ &= \frac{\mu(C) \mathbf{P}(\tilde{S}_\xi = \alpha(x, y)) \mathbf{P}(\tilde{S}_\xi = y')}{\mathbf{P}(\tilde{S}_\xi \in C) \mathbf{P}(\tilde{S}_\xi = y)} \\ &= \mathbf{P}(\alpha(x, y)) \exp(\beta(y, y')), \end{aligned}$$

proving that B satisfies eq. (2.1) on page 3, and therefore that $\mathbf{P} \in \mathfrak{M}(\mathcal{D}, \mathcal{B})$. Remark that in this proof, we have taken advantage of the fact that the Markov substitute property is stable by conditioning. \square

Lemma 3.2

In the case when $\mathfrak{M}(\mathcal{D}, \mathcal{B}) = \mathfrak{M}(\mathcal{D}, \mathcal{B}')$, then $\mathcal{D}/\sim_{\mathcal{B}} = \mathcal{D}/\sim_{\mathcal{B}'}$.

PROOF. Assume that the hypothesis stated in the lemma is satisfied. According to the previous proposition, for any $C \in \mathcal{D}/\sim_{\mathcal{B}}$, there is $P \in \mathfrak{M}(\mathcal{D}, \mathcal{B})$ such that $\text{supp}(P) = C$. Since $P \in \mathfrak{M}(\mathcal{D}, \mathcal{B}')$, there is also $\mathcal{C}' \subset \mathcal{D}/\sim_{\mathcal{B}'}$ such that $C = \text{supp}(P) = \bigcup \mathcal{C}'$. Therefore $\mathcal{D}/\sim_{\mathcal{B}}$ is a coarser partition than $\mathcal{D}/\sim_{\mathcal{B}'}$. As \mathcal{B} and \mathcal{B}' play symmetric roles, the reverse is also true, so that the two partitions are equal, each being coarser than the other one. \square

We are now going to show that the set $\mathfrak{M}(\mathcal{D}, \mathcal{B})$ of \mathcal{B} -Markov processes on the domain \mathcal{D} forms an exponential family, although we will unfortunately do it in a non constructive way: we will not be able to provide an efficient algorithm to compute the corresponding energy function (or in other terms sufficient statistics). Moreover, we will restrict ourselves to the case when \mathcal{B} is a finite family of finite subsets of D^+ .

Definition 3.1

Given a domain $\mathcal{D} \subset D^+$, a set \mathcal{B} of subsets of D^+ and a subset $\mathcal{C} \subset \mathcal{D}/\sim_{\mathcal{B}}$ of components of $\mathcal{D}/\sim_{\mathcal{B}}$, define $\mathfrak{M}_{\mathcal{C}}(\mathcal{D}, \mathcal{B})$ as the set of \mathcal{B} -Markov probability measures on \mathcal{D} whose support is $\bigcup_{C \in \mathcal{C}} C$.

Proposition 3.3

Given any domain $\mathcal{D} \subset D^+$ —that may be infinite and may be D^+ itself—any finite set \mathcal{B} of finite subsets of D^+ , there is a finite set of pairs \mathcal{P} , that we can choose such that each one is included in a member of \mathcal{B} , such that the sets of \mathcal{B} -Markov and \mathcal{P} -Markov substitute processes on the domain \mathcal{D} are the same—that is such that $\mathfrak{M}(\mathcal{D}, \mathcal{B}) = \mathfrak{M}(\mathcal{D}, \mathcal{P})$. Moreover, since it is finite, we can if required choose \mathcal{P} to be minimal for the inclusion relation—meaning that removing a pair from \mathcal{P} would change $\mathfrak{M}(\mathcal{D}, \mathcal{P})$ to a broader model.

For any finite subset of components $\mathcal{C} \subset \mathcal{D}/\sim_{\mathcal{B}}$, let us define the set of active pairs as

$$\mathcal{A} = \left\{ \{y, y'\} \in \mathcal{P}, \text{ there is } x \in (D^*)^2 \text{ such that } \alpha(x, \{y, y'\}) \subset \bigcup_{C \in \mathcal{C}} C \right\}.$$

There is a non empty subset of pairs $\mathcal{F} \subset \mathcal{A}$, a matrix $(e_{i,j}, i \in \mathcal{F}, j \in \mathcal{A} \setminus \mathcal{F})$, a finite index set $\mathcal{I} = \mathcal{F} \cup \mathcal{C}$, and energy functions

$$\begin{aligned} U_i : \bigcup_{C \in \mathcal{C}} C &\rightarrow \mathbb{R}, \\ s &\mapsto U_i(s), \quad i \in \mathcal{I}, \end{aligned}$$

such that the set $\mathfrak{M}_{\mathcal{C}}(\mathcal{D}, \mathcal{B})$ is the linear exponential family

$$\mathfrak{M}_{\mathcal{C}}(\mathcal{D}, \mathcal{B}) = \left\{ P_{\beta}; \beta \in \mathfrak{B} \subset \mathbb{R}^{\mathcal{I}}, P_{\beta}(s) = Z_{\beta}^{-1} \exp\left(-\sum_{i \in \mathcal{I}} \beta_i U_i(s)\right), s \in \bigcup \mathcal{C} \right\},$$

$$\text{where } Z_{\beta} = \sum_{s \in \bigcup \mathcal{C}} \exp\left(-\sum_{i \in \mathcal{I}} \beta_i U_i(s)\right),$$

$$\text{and } \mathfrak{B} = \left\{ \beta \in \mathbb{R}^{\mathcal{I}}, Z_{\beta} < \infty \right\}.$$

Moreover, for any $\beta \in \mathfrak{B}$, the substitute exponent under P_{β} on \mathcal{D} of any pair $i = \{y_{i,0}, y_{i,1}\} \in \mathcal{F}$, indexed in a suitable way compatible with the definition of U_i , is given by

$$\beta(y_{i,0}, y_{i,1}) = \beta_i,$$

whereas the substitute exponent of $j \in \mathcal{A} \setminus \mathcal{F}$ is given by

$$\beta(y_{j,0}, y_{j,1}) = \sum_{i \in \mathcal{F}} \beta_i e_{i,j},$$

and the substitute exponent of $j \in \mathcal{D} \setminus \mathcal{A}$ can be arbitrarily set to any real value. On the other hand, the probabilities $(P_{\beta}(C), C \in \mathcal{C})$ are given by

$$P_{\beta}(C) = Z_{\beta}^{-1} \exp(\beta_C) \sum_{s \in C} \exp\left(-\sum_{i \in \mathcal{F}} \beta_i U_i(s)\right).$$

As a consequence, for any $\beta, \beta' \in \mathfrak{B}$,

$$P_{\beta'} = P_{\beta} \iff \begin{cases} \beta'_i = \beta_i, & i \in \mathcal{F}, \\ \beta'_C = \beta_C + \log(Z_{\beta'}/Z_{\beta}), & C \in \mathcal{C}. \end{cases}$$

PROOF. Let us start with the set of pairs

$$\mathcal{D}' = \left\{ \{y, y'\} \subset B \in \mathcal{B}, y \neq y' \right\}.$$

In view of the second statement of proposition 2.2 on page 3, the property that $P \in \mathfrak{M}(\mathcal{D}, \mathcal{B})$ can be reformulated as

$$P(\alpha(x, y')) = P(\alpha(x, y)) \exp(\beta(y, y')),$$

$$x \in (D^*)^2, (y, y') \in \bigcup_{B \in \mathcal{B}} B^2, \alpha(x, \{y, y'\}) \subset \mathcal{D},$$

for some global exponent function $\beta : \bigcup_{B \in \mathcal{B}} B^2 \rightarrow \mathbb{R}$. Since

$$\bigcup_{B \in \mathcal{B}} B^2 = \bigcup_{B \in \mathcal{P}'} B^2,$$

this shows that $\mathfrak{M}(\mathcal{D}, \mathcal{B}) = \mathfrak{M}(\mathcal{D}, \mathcal{P}')$.

Since \mathcal{B} is assumed to be a finite family of finite sets, \mathcal{P}' is a finite set of pairs and we can obtain if wanted a minimal set of pairs \mathcal{P} by removing redundant pairs from \mathcal{P}' .

Remark that according to lemma 3.2 on page 6, $\mathcal{D}/\sim_{\mathcal{B}} = \mathcal{D}/\sim_{\mathcal{P}}$.

For any $\mathcal{C} \subset \mathcal{D}/\sim_{\mathcal{B}}$, according to proposition 3.1 on page 5, the set $\mathfrak{M}_{\mathcal{C}}(\mathcal{D}, \mathcal{B})$ is non empty, and is equal to $\mathfrak{M}_{\mathcal{C}}(\mathcal{D}, \mathcal{P})$, by construction of \mathcal{P} .

Let us index the corresponding set of active pairs \mathcal{A} defined in the proposition as

$$\mathcal{A} = \{(y_{i,0}, y_{i,1}), 1 \leq i \leq I\}.$$

For any two states s and $s' \in C \in \mathcal{C}$, let us define the set of paths connecting s to s' as

$$\mathfrak{P}_{s,s'} = \left\{ (x_j, i_j, \sigma_j), 0 \leq j \leq L, L \in \mathbb{N}, x_j \in (D^*)^2, 1 \leq i_j \leq I, \sigma_j \in \{0, 1\} \right\},$$

such that

$$\begin{aligned} \alpha(x_0, y_{i_0, \sigma_0}) &= s, \\ \alpha(x_L, y_{i_L, 1-\sigma_L}) &= s', \\ \alpha(x_j, y_{i_j, \sigma_j}) &= \alpha(x_{j-1}, y_{i_{j-1}, 1-\sigma_{j-1}}) \in \mathcal{D}, \quad 0 < j \leq L. \end{aligned}$$

We see from the description of $\mathcal{D}/\sim_{\mathcal{P}}$ as the connected components of the graph $\left\{ (\alpha(x, y), \alpha(x, y')), x \in (D^*)^2, \{y, y'\} \in \mathcal{P} \right\} \cap \mathcal{D}^2$ defined by \mathcal{P} that $\mathfrak{P}_{s,s'} \neq \emptyset$ and that in fact

$$\alpha(x_j, y_{i_j, \sigma_j}) = \alpha(x_{j-1}, y_{i_{j-1}, 1-\sigma_{j-1}}) \in C, \quad 0 < j \leq L.$$

For any $\pi = (x_j, i_j, \sigma_j)_{0 \leq j \leq L} \in \mathfrak{P}_{s,s'}$, let

$$U_i(\pi) = \sum_{j=0}^L \mathbb{1}(i_j = i) (2\sigma_j - 1).$$

Let us choose for any $C \in \mathcal{C}$ a reference state s_C , and consider the set of loops $\mathfrak{L} = \bigcup_{C \in \mathcal{C}} \mathfrak{P}_{s_C, s_C}$. Consider the I functions

$$\begin{aligned} U_i : \mathfrak{L} &\rightarrow \mathbb{R}, \\ \pi &\mapsto U_i(\pi), \end{aligned} \tag{3.5}$$

where $1 \leq i \leq I$. Reindexing the set of pairs if necessary, assume that U_k , $K < k \leq I$ is a maximum free subset of $(U_i, 1 \leq i \leq I)$, so that there is a matrix $e_{i,j}$, such that

$$U_i = - \sum_{k=K+1}^I e_{i,k} U_k, \quad 1 \leq i \leq K. \quad (3.6)$$

(In the case when U_i , $1 \leq i \leq I$ are already linearly independent, it should be understood that $K = 0$ and that the above statement is void, since no index i satisfies $1 \leq i \leq 0$. Let us also remark that we can have $K = I$ in the case when all the functions U_i are equal to the null function.) For any set of parameters $\beta = (\beta_i, 1 \leq i \leq I) \in \mathbb{R}^I$, for any path $\pi = (x_j, i_j, \sigma_j)_{0 \leq j \leq L} \in \mathfrak{P}_{s,s'}$, let

$$w_\beta(\pi) = \sum_{j=0}^L (1 - 2\sigma_j) \beta_{i_j} = - \sum_{i=1}^I \beta_i U_i(\pi).$$

Lemma 3.4

For any $\beta \in \mathbb{R}^I$ such that

$$\beta_k = \sum_{i=1}^K \beta_i e_{i,k}, \quad K < k \leq I, \quad (3.7)$$

with the convention that in the case when $K = 0$, $\beta_k = 0$, $0 < k \leq I$, and in the case when $K = I$, the assumption is void, for any $C \in \mathcal{C}$, any $s \in C$, and any $\pi, \pi' \in \mathfrak{P}_{s_C, s}$,

$$w_\beta(\pi') = w_\beta(\pi).$$

PROOF. There is $\pi'' \in \mathfrak{P}_{s_C, s_C}$ such that $w_\beta(\pi'') = w_\beta(\pi') - w_\beta(\pi)$ (where π'' is built in an obvious way as the concatenation of π' and of the reverse of π). Equation (3.7) ensures that $w_\beta(\pi'') = 0$. Indeed in this case

$$\begin{aligned} w_\beta(\pi'') &= - \sum_{i=1}^I \beta_i U_i(\pi'') = \sum_{i=1}^K \sum_{k=K+1}^I \beta_i e_{i,k} U_k(\pi'') - \sum_{k=K+1}^I \beta_k U_k(\pi'') \\ &= \sum_{k=K+1}^I \left(\sum_{i=1}^K \beta_i e_{i,k} - \beta_k \right) U_k(\pi'') = 0. \quad \square \end{aligned}$$

For any $s \in C \in \mathcal{C}$, let us choose $\pi_s \in \mathfrak{P}_{s_C, s}$, and define

$$U_i(s) = U_i(\pi_s) + \sum_{k=K+1}^I e_{i,k} U_k(\pi_s), \quad 1 \leq i \leq K, \quad (3.8)$$

so that, when eq. (3.7) holds,

$$w_\beta(\pi_s) = \sum_{i=1}^K \beta_i U_i(s).$$

Let us index the set of components \mathcal{C} (assumed to be finite) as

$$\mathcal{C} = \{C_{K+1}, \dots, C_J\},$$

and define

$$U_j(s) = -\mathbf{1}(s \in C_j), \quad K < j \leq J.$$

Define the parameter set $\mathfrak{B} \subset \mathbb{R}^J$ as

$$\mathfrak{B} = \left\{ \beta \in \mathbb{R}^J, Z_\beta \stackrel{\text{def}}{=} \sum_{s \in \bigcup \mathcal{C}} \exp\left(-\sum_{j=1}^J \beta_j U_j(s)\right) < \infty \right\}.$$

For each $\beta \in \mathfrak{B}$, define $P_\beta \in \mathcal{M}_+^1(\bigcup \mathcal{C})$ as

$$P_\beta(s) = Z_\beta^{-1} \exp\left(-\sum_{j=1}^J \beta_j U_j(s)\right), \quad s \in \bigcup_{C \in \mathcal{C}} C.$$

Lemma 3.5

For any $\beta \in \mathfrak{B}$, $P_\beta \in \mathfrak{M}_{\mathcal{C}}(\mathcal{D}, \mathcal{P})$. Define

$$\beta'_k = \begin{cases} \beta_k, & 1 \leq k \leq K, \\ \sum_{i=1}^K \beta_i e_{i,k}, & K < k \leq I. \end{cases}$$

For any $i \in \{1, \dots, I\}$,

$$\beta(y_{i,0}, y_{i,1}) = \beta'_i$$

is the substitute exponent of $\{y_{i,0}, y_{i,1}\}$ for the Markov substitute measure P_β on \mathcal{D} . When $\{y, y'\} \in \mathcal{P} \setminus \mathcal{A}$ is not an active pair, its substitute exponent $\beta(y, y')$ is not uniquely defined and can be set to any arbitrary real value.

PROOF. First of all, it is immediate to see that $\text{supp}(P_\beta) = \bigcup \mathcal{C}$. Consider first any pair $\{y, y'\} \in \mathcal{P} \setminus \mathcal{A}$ and any $x \in (D^*)^2$ such that $\alpha(x, \{y, y'\}) \subset \mathcal{D}$. Since $\alpha(x, \{y, y'\}) \not\subset \bigcup \mathcal{C}$, and since $\alpha(x, y) \sim_{\mathcal{P}} \alpha(x, y')$, necessarily

$$\alpha(x, \{y, y'\}) \cap \left(\bigcup \mathcal{C}\right) = \emptyset,$$

so that $P_\beta(\alpha(x, y)) = P_\beta(\alpha(x, y')) = 0$ and

$$0 = P_\beta(\alpha(x, y')) = P_\beta(\alpha(x, y)) \exp(\beta(y, y')),$$

for any choice of $\beta(y, y') \in \mathbb{R}$. Consider any $i \in \{1, \dots, I\}$ and any $x \in (D^*)^2$, such that $z = \alpha(x, y_{i,0}) \in \mathcal{D}$ and $z' = \alpha(x, y_{i,1}) \in \mathcal{D}$. Since $z \sim_{\mathcal{D}} z'$, there is $C \in \mathcal{D}/\sim_{\mathcal{D}}$ such that $\{z, z'\} \subset C$. If $C \notin \mathcal{C}$, then $P_\beta(C) = P_\beta(z) = P_\beta(z') = 0$, so that obviously

$$0 = P_\beta(z') = P_\beta(z) \exp(\beta'_i).$$

Assume now on the other hand that $C \in \mathcal{C}$. Let π' be the concatenation of π_z (defined before eq. (3.8) on page 10) and $(x, i, 0)$. We see that $\pi' \in \mathfrak{P}_{s_C, z'}$, so that

$$-\sum_{j=1}^K \beta_j U_j(z') = w_{\beta'}(\pi_{z'}) = w_{\beta'}(\pi') = w_{\beta'}(\pi_z) + \beta'_i = -\sum_{j=1}^K \beta_j U_j(z) + \beta'_i.$$

Remark also that $U_j(z) = U_j(z')$, $K < j \leq J$, since z and z' belong to the same component $C \in \mathcal{C}$. Therefore

$$\begin{aligned} \log(P(z')) + \log(Z_\beta) &= -\sum_{j=1}^J \beta_j U_j(z') \\ &= -\sum_{j=1}^J \beta_j U_j(z) + \beta'_i = \log(P_\beta(z)) + \log(Z_\beta) + \beta'_i, \end{aligned}$$

proving that

$$P_\beta(z') = P_\beta(z) \exp(\beta'_i),$$

and therefore that $P_\beta \in \mathfrak{M}_{\mathcal{C}}(\mathcal{D}, \mathcal{P})$ with the prescribed substitute exponents. \square

Lemma 3.6

Let us put

$$Z_{\beta_{1:K}, j} = \sum_{s \in C_j} \exp\left(-\sum_{i=1}^K \beta_i U_i(s)\right),$$

where $\beta_{1:K} = \{\beta_1, \dots, \beta_K\}$, so that

$$Z_\beta = \sum_{j=K+1}^J \exp(\beta_j) Z_{\beta_{1:K}, j}.$$

The parameters $\beta_{(K+1):J} = \{\beta_{K+1}, \dots, \beta_J\}$ are related to P_β by the following relation

$$P_\beta(C_j) = \exp(\beta_j) \frac{Z_{\beta_{1:K}, j}}{Z_\beta}, \quad K < j \leq J.$$

PROOF. By definition of Z_β ,

$$Z_\beta = \sum_{s \in \bigcup \mathcal{C}} \exp\left(-\sum_{i=1}^J \beta_i U_i(s)\right) = \sum_{j=K+1}^J \sum_{s \in C_j} \exp\left(-\sum_{i=1}^J \beta_i U_i(s)\right).$$

Since $U_j(s) = -\mathbb{1}(s \in C_j)$, $K < j \leq J$,

$$Z_\beta = \sum_{j=K+1}^J \sum_{s \in C_j} \exp\left(\beta_j - \sum_{i=1}^K \beta_i U_i(s)\right) = \sum_{j=K+1}^J \exp(\beta_j) Z_{\beta_{1:K}, j}.$$

Moreover, the definition of P_β implies that

$$\begin{aligned} P_\beta(C_j) &= \sum_{s \in C_j} Z_\beta^{-1} \exp\left(-\sum_{i=1}^J \beta_i U_i(s)\right) \\ &= \sum_{s \in C_j} Z_\beta^{-1} \exp\left(\beta_j - \sum_{i=1}^K \beta_i U_i(s)\right) = \exp(\beta_j) \frac{Z_{\beta_{1:K}, j}}{Z_\beta}, \quad K < j \leq J. \quad \square \end{aligned}$$

Lemma 3.7

For any $\beta, \beta' \in \mathfrak{B}$

$$P_{\beta'} = P_\beta \iff \begin{cases} \beta'_i = \beta_i, & 1 \leq i \leq K, \\ \beta'_i = \beta_i + \log(Z_{\beta'}/Z_\beta), & K < i \leq J. \end{cases}$$

PROOF. This is a consequence of the two previous lemmas and the fact that $P \in \mathfrak{M}_{\mathcal{C}}(\mathcal{D}, \mathcal{P})$ is determined by the substitute exponents of active Markov substitute pairs and the probabilities

$$P(C_j) = \exp(\beta_j) \frac{Z_{\beta_{1:K}, j}}{Z_\beta}, \quad K < j \leq J,$$

that are themselves determined by P . The constant $\log(Z_{\beta'}/Z_\beta)$ is there just because we chose not to break the symmetry of the role played by the components C_j , $K < j \leq J$. Since $\sum_{j=K+1}^J P(C_j) = 1$, we could have characterized the vector of probabilities $(P(C_j))_{K < j \leq J}$ by only $J - K - 1$ parameters instead of $J - K$. In other words we could have used the fact that $U_J(s) = -1 - \sum_{j=K+1}^{J-1} U_j(s)$, to remove the parameter β_J from the representation. \square

Lemma 3.8

The reverse inclusion

$$\mathfrak{M}_{\mathcal{C}}(\mathcal{D}, \mathcal{B}) \subset \{P_\beta, \beta \in \mathfrak{B}\}$$

is also satisfied.

PROOF. Consider any probability measure $P \in \mathfrak{M}_{\mathcal{C}}(\mathcal{D}, \mathcal{B}) = \mathfrak{M}_{\mathcal{C}}(\mathcal{D}, \mathcal{P})$ (we know from proposition 3.1 on page 5 that $\mathfrak{M}_{\mathcal{C}}(\mathcal{D}, \mathcal{P}) \neq \emptyset$). Let

$$\beta'_i = \beta(y_{i,0}, y_{i,1}), \quad 1 \leq i \leq I,$$

where $\beta(y_{i,0}, y_{i,1})$ is the substitute exponents of $\{y_{i,0}, y_{i,1}\}$ under P on \mathcal{D} . From the Markov substitute property expressed by eq. (2.1) on page 3, we see that for any $s, s' \in C \in \mathcal{C}$, any $\pi \in \mathfrak{P}_{s,s'}$,

$$P(s') = P(s) \exp(w_{\beta'}(\pi)).$$

Therefore, for any $s \in C \in \mathcal{C}$,

$$P(s) = P(s_C) \exp(w_{\beta'}(\pi_s)) = \exp\left(-\sum_{i=1}^I \beta'_i U_i(\pi_s)\right) P(s_C)$$

and for any $\pi \in \mathfrak{L}$,

$$1 = \exp(w_{\beta'}(\pi)) = \exp\left(-\sum_{i=1}^I \beta'_i U_i(\pi)\right).$$

Using eq. (3.6) on page 10, we obtain that

$$\sum_{k=K+1}^I \left(\beta'_k - \sum_{i=1}^K \beta'_i e_{i,k} \right) U_k(\pi) = 0, \quad \pi \in \mathfrak{L},$$

so that

$$\beta'_k = \sum_{i=1}^K \beta'_i e_{i,k}, \quad K < k \leq I,$$

since the functions $(U_k, K < k \leq I)$ defined by eq. (3.5) on page 9 are linearly independent. Therefore

$$\sum_{i=1}^I \beta'_i U_i(\pi_s) = \sum_{i=1}^K \beta'_i U_i(s), \quad s \in \bigcup \mathcal{C}.$$

On the other hand, putting

$$\beta_j = \log(P(s_{C_j})), \quad K < j \leq J,$$

we obtain that

$$P(s_C) = \exp\left(-\sum_{j=K+1}^J \beta_j U_j(s)\right), \quad \text{for any } C \in \mathcal{C}.$$

Let us define

$$\beta_i = \beta'_i, \quad 1 \leq i \leq K.$$

For any $s \in C \in \mathcal{C}$, we obtain that

$$\begin{aligned} P(s) &= \exp\left(-\sum_{i=1}^I \beta'_i U_i(\pi_s)\right) P(s_C) \\ &= \exp\left(-\sum_{i=1}^K \beta'_i U_i(s) - \sum_{j=K+1}^J \beta_j U_j(s)\right) = \exp\left(-\sum_{j=1}^J \beta_j U_j(s)\right). \end{aligned}$$

Remark that with this choice of parameter β ,

$$Z_\beta = \sum_{s \in \bigcup \mathcal{C}} \exp\left(-\sum_{j=1}^J \beta_j U_j(s)\right) = \sum_{s \in \bigcup \mathcal{C}} P(s) = 1,$$

so that $P = P_\beta$. □

We obtain proposition 3.3 on page 7 by gathering the previous lemmas together and indexing directly \mathcal{P} and \mathcal{C} by themselves instead of using numerical indices as in the proofs. □

Remark that proposition 3.3 implies that the maximum likelihood estimator in $\mathfrak{M}_{\mathcal{C}}(\mathcal{D}, \mathcal{B})$ is an asymptotically efficient estimator of the parameters β_i , $i \in \mathcal{I}$. This property does not provide a practical estimator though, since the construction of the energy functions U_i , $i \in \mathcal{I}$ is not explicit, at least in the general case. It is nevertheless possible to approximate the maximum likelihood estimator without computing the energy functions explicitly, using a Monte-Carlo simulation algorithm that is proposed in [Mainguy, 2014, page 135] and will be further presented and analysed in another publication.

4 Examples

4.1 Some simple recursive structures

Let us give an example showing that a minimal set of pairs is not necessarily free, so that we can have $\mathcal{P} \neq \mathcal{F}$, and that the set of free pairs \mathcal{F} —and therefore the form of the energy—may depend on the support $\bigcup_{C \in \mathcal{C}} C$ of the Markov substitute process in a non trivial way.

On the three words dictionary $D = \{a, b, c\}$, consider the domain $\mathcal{D} = D^+$ and the family of subsets $\mathcal{B} = \{B_1, B_2\}$, where $B_1 = \{ab, a\}$ and $B_2 = \{bc, c\}$. Define

$$\begin{aligned} C_1 &= \{ab^n c, n \in \mathbb{N}\}, \\ C_2 &= \{b^m cab^n, m, n \in \mathbb{N}\}, \\ C_3 &= \{b^k cab^m cab^n, k, m, n \in \mathbb{N}\}. \end{aligned}$$

It is easy to check that $C_k \in D^+ / \sim_{\mathcal{B}}$, $1 \leq k \leq 3$, so that we may consider the three supports C_k , corresponding to $\mathcal{C}_k = \{C_k\} \subset D^+ / \sim_{\mathcal{B}}$.

In C_1 , we have the loop

$$ac = \alpha((\varepsilon, c), a) \rightarrow \alpha((\varepsilon, c), ab) = abc = \alpha((a, \varepsilon), bc) \rightarrow \alpha((a, \varepsilon), c) = ac,$$

inducing the constraint

$$\beta(a, ab) = \beta(c, bc),$$

so that

$$\mathfrak{M}_{\mathcal{C}_1}(D^+, \mathcal{B}) = \{P \in \mathcal{M}_+^1(C_1); P(ab^n c) = r(1-r)^n, r \in]0, 1[\}.$$

In this case we can choose the set of free pairs either equal to $\mathcal{F}(\mathcal{C}_1) = \{B_1\}$ or equal to $\mathcal{F}(\mathcal{C}_1) = \{B_2\}$.

In C_2 , there is no non trivial loop, so that the set of free pairs is $\mathcal{F}(\mathcal{C}_2) = \mathcal{B}$, and we get an exponential family with two parameters

$$\begin{aligned} \mathfrak{M}_{\mathcal{C}_2}(D^+, \mathcal{B}) &= \{P \in \mathcal{M}_+^1(C_2); \\ &P(b^m cab^n) = r_1 r_2 (1-r_1)^m (1-r_2)^n, r_1, r_2 \in]0, 1[\}. \end{aligned}$$

In C_3 , we have the same non trivial loop as in C_1 , imposing the constraint $\beta(a, ab) = \beta(c, bc)$, so that we can choose $\mathcal{F}(\mathcal{C}_3) = \{B_1\}$ or $\mathcal{F}(\mathcal{C}_3) = \{B_2\}$, and

$$\begin{aligned} \mathfrak{M}_{\mathcal{C}_3}(D^+, \mathcal{B}) &= \{P \in \mathcal{M}_+^1(C_3); P(b^k cab^m cab^n) = r(1-r)^{k+m+n}, \\ &k, m, n \in \mathbb{N}, r \in]0, 1[\}. \end{aligned}$$

Note also that $\mathfrak{M}_{\mathcal{C}_1}(D^+, \mathcal{B}) = \mathfrak{M}_{\mathcal{C}_1}(D^+, \{B_1\}) = \mathfrak{M}_{\mathcal{C}_1}(D^+, \{B_2\})$, so that \mathcal{B} is not a minimal set of pairs on \mathcal{C}_1 , but is a minimal set of pairs both on \mathcal{C}_2 and \mathcal{C}_3 . Therefore, in $\mathfrak{M}_{\mathcal{C}_3}(D^+, \mathcal{B})$, \mathcal{B} is a minimal set of pairs but is not a free set of pairs.

4.2 Links with Markov chains

Let us now consider another example, to show that Markov substitute processes contain Markov chains. Consider a finite state space D and the family of substitute sets

$$\mathcal{B} = \left\{ \alpha((a, b), D), (a, b) \in D^2 \right\}.$$

Lemma 4.1

The model $\mathfrak{M}(D^L, \mathcal{B})$ contains the law of all time homogeneous Markov chains (S_1, \dots, S_L) with positive transition matrix M , that is the law of all Markov chains (S_1, \dots, S_L) such that

$$\mathbb{P}(S_k = b \mid S_{k-1} = a) = M(a, b) > 0, \quad (a, b) \in D^2, 1 < k \leq L.$$

PROOF. If S is such a Markov chain, for any context $x \in (D^*)^2$ and any

$$(a, y, b), (a, y', b) \in \alpha((a, b), D) \in \mathcal{B},$$

it is easy to check that

$$\mathbb{P}[S = \alpha(x, (a, y', b))] > 0 \text{ if and only if } \mathbb{P}[S = \alpha(x, (a, y, b))] > 0.$$

In this case, we can write x as $x = (w_{1:k}, w_{k+4:L})$, where $0 \leq k \leq L - 3$, $w_{1:k} = (w_1, \dots, w_k) \in D^k$, and $w_{k+4:L} = (w_{k+4}, \dots, w_L) \in D^{L-k-3}$, with the convention that $w_{1:0} = w_{L+1:L} = \varepsilon$. We can then compute

$$\begin{aligned} \mathbb{P}[S = \alpha(x, (a, z, b))] \\ &= \mathbb{P}[S_{1:k+1} = \gamma(w_{1:k}, a)] M(a, z) M(z, b) \\ &\quad \times \mathbb{P}[S_{k+4:L} = w_{k+4:L} \mid S_{k+3} = b]. \end{aligned}$$

Therefore

$$\mathbb{P}[S = \alpha(x, (a, y', b))] = \mathbb{P}[S = \alpha(x, (a, y, b))] \exp[\beta((a, y, b), (a, y', b))],$$

where

$$\beta((a, y, b), (a, y', b)) = \log \left(\frac{M(a, y') M(y', b)}{M(a, y) M(y, b)} \right),$$

proving that $\mathbb{P}_S \in \mathfrak{M}(D^L, \mathcal{B})$. □

Lemma 4.2

$$D^L / \sim_{\mathcal{B}} = \left\{ \alpha((a, b), D^{L-2}), (a, b) \in D^2 \right\}.$$

PROOF. It is easy to see that $\alpha((a, b), D^{L-2})$ is connected by the graph $\mathcal{G}(D^L, \mathcal{B})$ (this notation was defined in eq. (3.1) on page 4). On the other hand, if $(w_{1:L}, w'_{1:L}) \in \mathcal{G}(D^L, \mathcal{B})$, then $w_1 = w'_1$ and $w_L = w'_L$, showing that there is no connection between $\alpha((a, b), D^{L-2})$ and its complement in D^L . \square

Lemma 4.3

For any random process $S \in D^L$ such that $\mathbb{P}_S \in \mathfrak{M}(D^L, \mathcal{B})$, there is a time-homogeneous Markov chain (X_1, \dots, X_L) with positive transition matrix M , such that for any $(a, b) \in D^2$, such that $\mathbb{P}(S_1 = a, S_L = b) > 0$,

$$\mathbb{P}_{S|S_1=a, S_L=b} = \mathbb{P}_{X|X_1=a, X_L=b},$$

whereas the marginal law of the pair of end points $\mathbb{P}_{(S_1, S_L)}$ may be any arbitrary probability measure. On the other hand, the set of possible values of the probability measure \mathbb{P}_{X_1, X_L} is constrained by the relation

$$\mathbb{P}(X_L = b | X_1 = a) = M^{L-1}(a, b).$$

PROOF. In fact one can see from the definition of Markov substitute sets, that for this specific choice of \mathcal{B} , the model $\mathfrak{M}(D^L, \mathcal{B})$ is the set of one dimensional random fields with prescribed boundary conditions. Building on this remark, a slight modification of the proof that a stationary one dimensional random field with a finite state space is a stationary Markov chain gives the result stated in the lemma. For the sake of completeness, we give here a proof adapted from [Georgii, 1988, page 45].

Let S be as described in the lemma, and β its substitute exponent. Let c in D be some word of the dictionary. From the existence of the loop

$$\begin{aligned} cac^3 &= \alpha((c, c), acc) \rightarrow cayc^2 = \alpha((ca, \varepsilon), ycc) \\ &\rightarrow caybc = \alpha((c, c), ayb) \rightarrow cay'bc = \alpha((ca, \varepsilon), y'bc) \\ &\rightarrow cay'cc = \alpha((c, c), ay'c) \rightarrow cac^3, \end{aligned}$$

we deduce that

$$\beta(ac^2, ayc) + \beta(y c^2, ybc) + \beta(ayb, ay'b) - \beta(y'c^2, y'bc) - \beta(ac^2, ay'c) = 0,$$

so that, for any $(a, y, y', b) \in D^4$,

$$\beta(ayb, ay'b) = \beta(ac^2, ay'c) + \beta(y'c^2, y'bc) - \beta(ac^2, ayc) - \beta(y'c^2, ybc). \quad (4.1)$$

This means that all the substitute exponents are determined by the subfamily of substitute exponents consisting in

$$\beta(ac^2, abc), \quad (a, b) \in D^2.$$

Consider the positive matrix

$$A(a, b) = \exp[\beta(ac^2, abc)], \quad (a, b) \in D^2.$$

According to the Perron-Frobenius theorem, it has a unique positive eigenvector $(\psi(a) > 0, a \in D)$ of norm $\|\psi\| = 1$ associated to a real positive eigenvalue λ (which turns out to be its spectral radius). Introduce the matrix

$$M(a, b) = \lambda^{-1} \psi(a)^{-1} A(a, b) \psi(b).$$

and remark that it is a positive Markov transition matrix, due to the fact that ψ is a positive eigenvector with eigenvalue λ . We see from eq. (4.1) that

$$\beta(ayb, ay'b) = \log \left(\frac{M(a, y') M(y', b)}{M(a, y) M(y, b)} \right), \quad (a, b, y, y') \in D^4.$$

Let (X_1, \dots, X_L) be a Markov chain with transition matrix M and initial distribution some (arbitrary) probability measure on D with full support. The previous equation shows that $\mathbb{P}_X \in \mathfrak{M}(D^L, \mathcal{B})$, with the same substitute exponents as \mathbb{P}_S . From our study of Markov substitute processes, we know that the substitute exponents define the conditional distribution of a Markov substitute process on each component of $D^L / \sim_{\mathcal{B}}$ of positive probability, these components being described in the previous lemma. We conclude that for any $(a, b) \in D^2$ such that $\mathbb{P}[S \in \alpha((a, b), D^{L-2})] > 0$, or in other words such that $\mathbb{P}(S_1 = a, S_L = b) > 0$,

$$\mathbb{P}_{S|S \in \alpha((a, b), D^{L-2})} = \mathbb{P}_{X|X \in \alpha((a, b), D^{L-2})},$$

that can also be written as

$$\mathbb{P}_{S|S_1 = a, S_L = b} = \mathbb{P}_{X|X_1 = a, X_L = b}. \quad \square$$

This study shows that the substitute sets of Markov chains have a very specific structure, and therefore that Markov substitute processes form a much richer family of models than Markov chains, while they can still be parametrized as exponential families, ensuring that they have some valuable properties as a statistical model.

5 Multi-dimensional extensions

In this paper we have defined one-dimensional Markov substitute processes and shown that they are an extension of one-dimensional Markov random fields. We can also generalize the notion of a multi-dimensional Markov random field by proposing a definition for multi-dimensional Markov substitute processes.

Let us define first a notion of Markov substitute process indexed by an arbitrary finite set I .

Definition 5.1

Given a random process $S \in D^I$ indexed by a finite set I , we will say that (J, B) , where $J \subset I$ and $B \subset D^J$ is a Markov substitute set when there exists for any $y, y' \in B$, any $x \in D^{I \setminus J}$ a skew-symmetric substitute exponent $\beta_J(y, y') \in \mathbb{R}$ such that

$$\mathbb{P}(S_J = y', S_{I \setminus J} = x) = \mathbb{P}(S_J = y, S_{I \setminus J} = x) \exp[\beta_J(y, y')].$$

When $I \subset \mathbb{Z}^d$ is part of a d -dimensional lattice, one can make the definition translation invariant by imposing that for any $J \subset I$, (J, B) is a translation invariant Markov substitute set if and only if, for any $t \in \mathbb{Z}^d$ such that $t + J \subset I$, $(t + J, B \circ \tau_t)$ is a Markov substitute set in the sense of the above definition, where $\tau_t(i) = i - t$, and the substitute exponents are the same in the sense that

$$\beta_{t+J}(y \circ \tau_t, y' \circ \tau_t) = \beta_J(y, y').$$

It is easy to see that an obvious reformulation of proposition 3.3 on page 7 remains true for these two variants of the definition of Markov substitute sets. (We could also formulate analogous definitions for a process defined on a restricted domain $\mathcal{D} \subset D^I$.)

Remark however that these multi-dimensional variants are not properly speaking extensions of the one-dimensional setting, since in the one dimensional case, we can let the Markov substitute sets contain expressions of varying lengths, leading to the modeling of recursive structures. This ability of modeling recursive structures gives a special interest to one-dimensional Markov substitute processes.

6 Conclusion

We presented here a slightly more general definition of Markov substitute processes than in [Mainguy, 2014], where it is assumed most of the time that $\mathcal{D} = D^+$. We showed the main property of the model, namely that it is for each legitimate choice of support an exponential family. One can show a host of interesting additional properties, some depending on further assumptions on the domain \mathcal{D} . The model, noticeably, can be viewed as an extension of Markov chains and has deep

connections with context free grammars [Chomsky, 1956, Chi and Geman, 1998, Chi, 1999]. One can also propose algorithms to select Markov substitute models, estimate their parameters, simulate from them or compute the probability of a given sentence $s \in D^+$. We refer to [Mainguy, 2014] and to forthcoming publications for more information and insight on Markov substitute processes, a model at the crossroad of statistics and formal grammars.

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